CHE 221
Simulation Lab 5

03/04/2025

Departure functions for real fluids

Question 1:

1. You are given a file (`PV_data.csv`) containing PV (P in atm and V in Litres) data measured at 300 K for 1 mole of a gas. Read it using `readtable()` and extract P and V values. You can extract Pressure and Volume data as follows: P = data.Pressure_atm and V = data.Volume_L. (5 points)

2. Fit the Van der Walls equation of state to the PV data using `lsqcurvefit()` and obtain values of `a` and `b`. Use $R = 0.0821$ L·atm/(mol·K). Recall the formula of the Van der Walls equation:

$$P = \frac{RT}{(V - b)} - \frac{a}{V^2}. \tag{1}$$

   Plot the fit curve with the data. Hint: search for lsqcurvefit in the documentation and follow the first example, 'Single Exponential Fit'. (20 points)

3. Using the fit values plot isotherms on the PV plot at 200 K, 300 K, 350 K, and 400 K. (15 points)

Question 2: (40 points)

Use the Van der Walls equation of state from Q1 to plot enthalpy departure functions vs. ρ at 200 K, 300 K, 350 K, and 400 K, with ρ ranging from 0 to 10 mol/m^3.The enthalpy departure function is as follows:

$$\frac{H - H_{\text{ig}}}{RT} = \int_0^{\rho} -T \left(\frac{dZ}{dT}\right)_{\rho} \frac{d\rho}{\rho} + Z - 1. \tag{2}$$

Here, $Z = \frac{PV}{RT}$. Note, you can approach this question in a few different ways, and all correct solutions will receive full points.